trans-Chrysanthemol

Other names: ((1R,3R)-2,2-Dimethyl-3-(2-methylprop-1-en-1-yl)cyclopropyl)methanol-rel-
Inchi: InChI=1S/C10H18O/c1-7(2)5-8-9(6-11)10(8,3)4/h5,8-9,11H,6H2,1-4H3/t8-,9-/m1/s1
InchiKey: HIPIENNKVJCMAP-RKDXNWHRSA-N
Formula: C10H18O
SMILES: CC(C)=CC1C(CO)C1(C)C
Mol. weight [g/mol]: 154.25
CAS: 18383-58-9

Physical Properties

Property code	Value	Unit	Source
gf	8.01	kJ/mol	Joback Method
hf	-247.17	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	52.72	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.217		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1163.40		NIST Webbook
tb	522.06	K	Joback Method
tc	706.96	K	Joback Method
tf	277.60	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.21	J/mol×K	522.06	Joback Method
cpg	364.49	J/mol×K	552.88	Joback Method
cpg	377.93	J/mol×K	583.69	Joback Method
cpg	390.63	J/mol×K	614.51	Joback Method
cpg	402.69	J/mol×K	645.32	Joback Method
cpg	414.18	J/mol×K	676.14	Joback Method
cpg	425.20	J/mol×K	706.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18383589&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume